=> d his

(FILE 'HOME' ENTERED AT 07:33:40 ON 15 FEB 2000) FILE 'CA' ENTERED AT 07:33:49 ON 15 FEB 2000 3520 S ISOTOP? (5A) (TAG OR TAGANT OR TRACER OR SPIKE OR SPIKING OR LABEL) L111754 S (SPECIE OR ION OR CHROMIUM OR CR3 OR CR4 OR CRIII OR CR OR CRIV) (7A) L2(CONVER? OR INTERCONVER? 4 S L1 AND L2 L3L46704 S ISOTOP? (3A) DILUT? L5 330 S L1 AND L4 L6 19 S L2 AND L4 L7 11 S L5 AND (ALGOR? OR SPECIAT? OR INTERCHANG?) L861 S L5 AND(SOIL OR MEMORY OR NICKEL OR VANADIUM OR CHROMIUM OR OPTIM?) L9 86 S L3, L6-8 Æd 19 bib,ab 1-86 80 ANSWER 22 OF 86 CA COPYRIGHT 2000 ACS ΑN CA ΤI Nickel metabolism in humans investigated with an oral stable isotope AU Patriarca, Marina; Lyon, Thomas David B.; Fell, Gordon S. CS Clin. Biochem. Dep., Ist. Super. Sanita, Rome, Italy SO Am. J. Clin. Nutr. (1997), 66(3), 616-621 CODEN: AJCNAC; ISSN: 0002-9165 DTJournal LA English AB We report the results of the first complete study of nickel metab. in human subjects using a stable nickel isotope (62Ni) as tracer. Four healthy adult subjects (two women and two men) fasted overnight before ingesting 10  $\mu$ g 62Ni/kg body wt. Blood samples were drawn after fixed intervals of time and the total daily output of urine and feces was collected for the first 5 d after dose ingestion. 62Ni in plasma, urine, and feces was detd. by isotope-diln. inductively coupled plasma-mass spectrometry with 61Ni. The direct measurement of the fecal excretion of the tracer allowed a reliable assessment of nickel absorption from the gastrointestinal tract and we found no evidence of the excretion of absorbed nickel via the qut. percentage absorption calcd. from the amt. of 62Ni excreted in the feces ranged from 29% to 40%. Urinary excretion over 5 d ranged from 51% to 82% of the absorbed dose. Plasma 62Ni peaked between 1.5 and 2.5 h after ingestion and decreased by a factor of > 10 over the next few days. obsd. low between-subject variability of nickel absorption and excretion. Confounding factors such as contamination and dietary intake of nickel, which hampered earlier measurements in subjects dosed with naturally abundant nickel, were eliminated by using the tracer isotope 62Ni.

ANSWER 24 OF 86 CA COPYRIGHT 2000 ACS

127:214148 CA

TI Boron determination - a review of analytical methods

ΑU Sah, R. N.; Brown, P. H.

CS Department of Pomology, University of California, Davis, CA, 95616, USA SO

Microchem. J. (1997), 56(3), 285-304 CODEN: MICJAN; ISSN: 0026-265X

DTJournal; General Review

LA English

₩9

AN

AB A review with 175 refs. This paper reviews published methods of sample prepn., determinand purifn., and the detn. of boron concn. and isotopic compn. in a sample. The most common methods for the detn. of B concn. are spectrophotometric and plasma-source spectrometric methods. Although most spectrophotometric methods are based on colorimetric reactions of B with azomethine-H, curcumin, or carmine, other colorimetric and fluorometric

methods also were used to some extent. These methods, in general, suffer from numerous interferences and have low sensitivity and precision. Application of nuclear reaction and at. emission/absorption spectrometric (AES/AAS) methods has remained limited because these methods have poor sensitivity and suffer from serious memory effects and interferences. Among a large no. of published nuclear reaction methods only prompt- $\gamma$ spectrometry was of practical use. The prompt- $\gamma$  method can det. B concn. in intact samples, which makes this method esp. useful for some medical applications, including boron neutron capture therapy. However, this is a time-consuming method and not suitable for detection of low levels of B. Inductively coupled plasma optical emission spectrometry (ICP-OES) created a new dimension in B detn. because of its simplicity, sensitivity, and multielement capability. However, it suffers interferences and is not adequately sensitive for some nutritional and medical applications involving animal tissues that are naturally low in B. All methods involving the measurement of B isotopic compn. require a mass spectrometer. ionization mass spectrometry (TIMS) and secondary ion mass spectrometry (SIMS) were used to measure isotopic compn. of B; however, these methods are time consuming and require extensive sample prepn. and purifn. Development of inductively coupled plasma mass spectrometry (ICP-MS) not only overcame most of the drawbacks of earlier methods, but also its capability of measuring B isotopes made possible (1) B concn. detn. by isotope diln., (2) verification of B concn. by isotope fingerprinting in routine anal., and (3) detn. of total B concn. and B isotope ratio for biol. tracer studies in the same run. Therefore, plasma source MS appears to be the method of choice among present-day technologies.

- L9 ANSWER 25 OF 86 CA COPYRIGHT 2000 ACS
- AN 127:70460 CA
- TI Online Isotope Dilution Analysis with ICPMS Using Reverse Flow Injection
- AU Beauchemin, Diane; Specht, August A.
- CS Department of Chemistry, Queen's University, Kingston, ON, K7L 3N6, Can.
- SO Anal. Chem. (1997), 69(16), 3183-3187 CODEN: ANCHAM; ISSN: 0003-2700
- DT Journal
- LA English
- A simple flow injection manifold is described to perform the addn. of AB isotopic spikes to aq. samples online with inductively coupled plasma mass spectrometry (ICPMS). The anal. involves one multielement spike injection in the sample carrier and another injection of the spike soln. in a std. carrier. This std. must contain one element which is not present in the spike soln., to allow the detn. of the dispersion coeff. The same std. also allows a reverse isotope diln. (ID) anal., in addn. to corrections for mass discrimination and any spectroscopic interference on one of the two isotopes used for the ID anal. This flow injection approach, therefore, requires only one isotope free of spectroscopic interference for elements whose isotopic distribution does not vary in nature (two isotopes are still needed for other elements since the "natural" ratio must then also be detd.). No preliminary anal. of the sample is required prior to the actual ID anal. Furthermore, the concn. profile resulting from the flow injection allows the selection of the best isotopic ratio in terms of error propagation. This approach, therefore, makes ID anal. as simple as an external calibration but with added accuracy and precision. successfully applied to the anal. of a river water certified ref. material and to saline water.
- L9 ANSWER 26 OF 86 CA COPYRIGHT 2000 ACS
- AN 127:64716 CA
- TI Determination of trace elements in rice flour by isotope dilution

inductively coupled plasma mass spectrometry

AU Park, Chang J.; Suh, Jung K.

- CS Korea Research Institute of Standards and Science, Taejon, 305-600, S. Korea
- SO J. Anal. At. Spectrom. (1997), 12(5), 573-577 CODEN: JASPE2; ISSN: 0267-9477
- DT Journal
- LA English
- Two rice flour ref. materials (normal and elevated trace concns.) were AB prepd. from brown rice produced in Korea. As part of the certification process, trace elements such as Cr, Fe, Cd and Pb were detd. by an isotopic diln. ICP-MS method. About 0.4 g of rice flour samples spiked with appropriate amts. of enriched spike isotopes was decompd. in high-pressure microwave digestion bombs. For the detn. of Cr and Fe, the ICP-MS instrument employed in the present work was operated under cool plasma conditions. The cool plasma was generated by inserting a copper shield between the load coil and the plasma, and by increasing the aerosol carrier gas flow rate up to 1.31 min-1. An approx.  $\mu$ g ml-1 Ca matrix in the digested soln. was obsd. to induce serious spectral interference on the detn. of Fe; hence, the Ca matrix was sepd. from the analyte using a microcolumn loaded with silica-immobilized 8-hydroxyquinoline. results for National Institute of Stds. and Technol. Std. Ref. Material 1568, Japan National Institute for Environmental Studies Certified Ref. Material 10-a and Korea Research Institute of Stds. and Science ref. materials are presented together with detection limits.
- ANSWER 28 OF 86 CA COPYRIGHT 2000 ACS
- AN 125:315520 CA
- TI Determination of lithium as a chemical tracer and its application to flow rate measurements
- AU Park, Chang J.
- CS Korea Res. Inst. Standards Science, Taejon, 305-600, S. Korea
- SO Analyst (Cambridge, U. K.) (1996), 121(9), 1311-1316 CODEN: ANALAO; ISSN: 0003-2654
- DT Journal
- LA English
- AB An isotope diln. equation is derived whereby the spike concn. is calibrated through so-called reverse isotope diln. with the primary std. soln. It is also demonstrated that potential systematic errors due to false spike enrichment values and the mass bias effect are minimized provided that spike addns. are judiciously controlled so that the isotope ratio of the spiked primary std. soln. does not differ from those of the spiked samples by more than 20%. Lithium was used as a chem. tracer to measure flow rates in an exptl. test facility. Thirty-two samples were collected downstream of the injection point and analyzed by isotope diln. ICP-MS. Six expts. were carried out on Sept. 28 and Nov. 8, 1995, to measure flow rates by the chem. tracer method. By optimizing the exptl. conditions, the chem. tracer method gave flow rates that differed by <0.4% from the ref. value.
  - ANSWER 32 OF 86 CA COPYRIGHT 2000 ACS
- AN 124:20548 CA
- TI Determination of Picogram Quantities of Vanadium in Calcite and Seawater by Isotope Dilution Inductively Coupled Plasma Mass Spectrometry with Electrothermal Vaporization
- AU Hastings, David W.; Emerson, Steven R.; Nelson, Bruce K.
- CS School of Oceanography, University of Washington, Seattle, WA, 98195, USA
- SO Anal. Chem. (1996), 68(2), 371-7 CODEN: ANCHAM; ISSN: 0003-2700
- DT Journal

LA English

The authors developed a method to measure picogram quantities of V in AB calcite and seawater by isotope diln. (ID) inductively coupled plasma mass spectrometry using electrothermal vaporization (ETV) to introduce the sample into the plasma. A 50V isotope spike enriched to 44 atom % was equilibrated with samples, followed by chem. purifn. by cation exchange Samples were introduced into the ETV unit with a Pd modifier and heated to 1000°. This quant. eliminates the ClO+ isobaric interference with V at m/z 51 for solns. up to 0.5 N HCl. The procedural blank was 0.27 pg of V. Corrections for 50Ti and 50Cr, which interfere with the 50V signal, were made by measurement of 49Ti and 53Cr. These isobaric interferences and variable ArC levels were the limiting sources of error in the ID measurement and diminished the detection limit to 6 pg of V. detection limit for nonisotope diln. applications was 0.3 pg of V. Measurement precision on the same sample of dissolved calcite over one run was  $\pm 3\%$  (1 $\sigma$ ). Accuracy was confirmed by detn. of V stds. in CaCO3 and by comparative measurement with ID thermal ionization mass spectrometry and graphite furnace at. absorption spectroscopy.

- L9 ANSWER 33 OF 86 CA COPYRIGHT 2000 ACS
- AN 123:264623 CA
- TI Iodine speciation in size fractionated atmospheric particles by isotope dilution mass spectrometry
- AU Wimschneider, Andrea; Heumann, Klaus G.
- CS Inst. Anorganische Chemie, Univ. Regensburg, Regensburg, D-93040, Germany
- SO Fresenius' J. Anal. Chem. (1995), 353(2), 191-6 CODEN: FJACES; ISSN: 0937-0633
- DT Journal
- LA English
- AB An isotope diln. mass spectrometric method has been developed for the accurate and sensitive detn. of I- and IO3- in atm. aerosol particulates. The direct I speciation has been possible by the use of species, specifically 129I enriched spike solns. and sepn. of the isotope dild. species by anion exchange chromatog. after water extn. of the filters. Size fractionated collection of aerosol particles by a six stage impactor system shows different distributions of I- and IO3- for particles of different size with specific patterns for anthropogenically influenced continental and unpolluted marine aerosols, resp. The detection limit for particulate I- and IO3- has been (3-5) pg/m3 for sampling vols. of 3000 m3. Oil used for heating plants could be identified as one but not the only anthropogenic I source.
- LY ANSWER 40 OF 86 CA COPYRIGHT 2000 ACS
- AN 121:147789 CA
- TI Error Propagation in Isotope Dilution Analysis As Determined by Monte Carlo Simulation
- AU Patterson, K.Y.; Veillon, C.; O'Haver, T. C.
- CS Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, 20742, USA
- SO Anal. Chem. (1994), 66(18), 2829-34 CODEN: ANCHAM; ISSN: 0003-2700
- DT Journal
- LA English
- AB Error propagation in isotope diln. anal. (IDA) can be studied with Monte Carlo (MC) simulation. In inductively coupled plasma mass spectrometry with ion-counting detection, the limiting error in the measured isotope ratio can be described with Poisson statistics. Taking into account this error in the measured isotope ratio, parameters for IDA can be optimized. The utility of MC simulation for IDA is illustrated in the optimization of

conditions for Zn anal. The min. imprecision in the detn. of Zn by IDA was found for the internal std. enriched with the isotope having the lowest natural abundance. In addn. to optimizing anal. conditions, MC simulation can provide information on the theor. detection limits in double and triple IDA for stable isotope tracers.

LO ANSWER 45 OF 86 CA COPYRIGHT 2000 ACS

AN 120:158076 CA

- TI Determination of Natural and Isotopically Enriched Chromium in Urine by Isotope Dilution Gas Chromatography/Mass Spectrometry
- AU Veillon, Claude; Patterson, Kristine Y.; Rubin, Michelle A.; Moser-Veillon, Phylis B.
- CS Vitamin and Mineral Nutrition Laboratory, Beltsville Human Nutrition Research Center, Beltsville, MD, 20705, USA
- SO Anal. Chem. (1994), 66(6), 856-60 CODEN: ANCHAM; ISSN: 0003-2700

DT Journal

LA English

AB A volatile chelate is formed with trifluoroacetylacetone (TFA) and the fragment ions corresponding to Cr(TFA)2+ in the 356-360 m/z region are monitored. The chelate is thermally stable and exhibits no memory effects when isotope ratios change. The detection limit for the method is 0.03 ng Cr/g, and the accuracy is verified by certified ref. materials and by an independent method. The method is highly specific for chromium, due to the combined properties of the chelating agent, chromatog. column, and mass-specific detector. In addn. to total chromium detns., the method can also be used to quantitate enriched stable isotopes of chromium used as metabolic tags in tracer expts. in human nutrition studies.

ANSWER 46 OF 86 CA COPYRIGHT 2000 ACS

117:239331 CA

- TI Determination of iron and ten other trace elements in the Open Ocean Seawater reference material NASS-3 by inductively coupled plasma mass spectrometry
- AU Akatsuka, Kunihiko; McLaren, James W.; Lam, Joseph W.; Berman, Shier S. CS Inst. Environ. Chem., Natl. Res. Counc. Canada, Ottawa, ON, K1A OR6, Can.
- SO J. Anal. At. Spectrom. (1992), 7(6), 889-94 CODEN: JASPE2; ISSN: 0267-9477

DT Journal

LA English AB Fe and

Fe and 10 other trace elements were detd. in the Open Ocean Seawater certified ref. material NASS-3 by inductively coupled plasma mass spectrometry after sepn. and concn. on silica-immobilized 8-hydroxyquinoline. Fe and Mo were sepd. after adjustment the samples to pH 3 prior to passage through the column, whereas for the other 9 elements preconcn. was performed at pH 8. Detn. of Fe by isotope diln., with 56Fe as the ref. isotope and 57Fe as the spike, required the use of a N-Ar mixed-gas plasma with partial aerosol desolvation. The detection limits of the method, based on a 90-fold preconcn., range 0.04 n/g-dm3 for U to 6.3 ng/dm3 for Zn.

ANSWER 52 OF 86 CA COPYRIGHT 2000 ACS

N 115:154049 CA

- TI Mass isotopomer analysis: theoretical and practical considerations AU Lee, W. N. Paul; Byerley, Lauri O.; Bergner, E. Anne; Edmond, John
- CS Dep. Pediatr., Harbor, UCLA Med. Cent., Torrance, CA, 90509, USA
- SO Biol. Mass Spectrom. (1991), 20(8), 451-8 CODEN: BIMSEH; ISSN: 1052-9306
- DT Journal; General Review
- LA English
- AB A review, with 17 refs., on a theory of mass isotopomer anal. based on the well-known principle of isotope diln. mass spectrometry. An algorithm for

the detn. of isotope incorporation into a metabolic substrate from a labeled precursor using mass isotopomer anal. is presented. The steps include the detn. of the contribution of the derivatization reagent to the obsd. spectrum of the derivatized substrate and the correction of contribution from 13C natural abundance using multiple linear regression anal. Examples of the application of this theory to det. the spectrum of the trimethylsilyl deriv. of the pure unlabeled or mononuclidic cholesterol, and the calcn. of mass isotopomer distribution in cholesterol due to tracer incorporation using this pure unlabeled spectrum, are also provided.

ANSWER 85 OF 86 CA COPYRIGHT 2000 ACS

AN 69:40955 CA

TI Determination of trace amounts of chromium by stable isotope-dilution mass spectrometry

AU Hedley, A.

CS Bragg Lab., Nav. Ordnance Insp. Estab., Sheffield, Engl. SO Analyst (London) (1968), 93(1106), 289-91 CODEN: ANALAO

DT Journal

LA English

Cr (0.003-0.2%) in steel, Cu-base alloys, and Al-base alloys was detd. by AΒ stableisotope diln. mass spectrometry. To prep. the tracer soln., fuse 2.5 g. Cr203, which is artifically enriched with 97.5% 53Cr, with a 10-fold excess of 2:1 Na2CO3-KNO3. Leach the melt with H2O, add dropwise a slight excess of 5% Pb(NO3)2, and allow to stand 30 min. at room temp. Centrifuge and wash the ppt. 10 times with H2O. Dissolve the ppt. in HNO3 (sp. gr. 1.42) and dil. to 50 ml. so that 1 ml. is equiv. to ~30  $\gamma$  53Cr. Dissolve the sample and 0.5 ml. of tracer soln. (a 1:1 isotopic ratio is preferred) in 10 ml. HCl and oxidize with a few drops of HNO3. Fume the soln. with 10 ml. of 50% H2SO4, cool, dil. to ~50 ml., add 2 ml. 10% Ce(SO4)2, and boil Cool the soln. to room temp., make the soln. N in HGl, and ext. 1 Wash the org. layer with four 25-ml. portions min. with 20 ml. MeCOBu-iso. of N HCl before back extg. Cr with two 10-ml. portions of H2O. Evap. the aq. soln. to the smallest possible vol. for the mass spectrometric anal. Several standards were analyzed [sample, % Cr present, % Cr found, given:] steel, 0.039, 0.039; steel, 0.045, 0.043; Al alloy, 0.06, 0.061-0.066; Al alloy, 0.24, 0.242; Cu alloy, 0.35, 0.035-0.037.

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     9961 S BALANCE(2A) (MASS OR SPECIE)
L1
    16084 S (STABLE OR DILUT?) (2A) ISOTOP?
L2
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      161 S L1 AND L2
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      132 S L3 NOT PY>1997
     7203 S L1/TI OR L2/TI
L5
       61 S L4 AND L5
L6
       44 S L4 AND (REDOX OR REACTION OR REDUCTION OR OXIDAT? OR OXIDIZ? OR
L7
          INTERCOVER?)
L8
       92 S L6-7
       40 S L4 NOT L8
L9
       3 S L9 AND CHROM?
L10
L11
       2 S L10 AND GAS
       94 S L8, L11
L12
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=> d 112 bib, ab 1-94

ANSWER 10 OF 94 CA COPYRIGHT 2000 ACS L12

AN 126:92288 CA

TIA model of isotope fractionation in reacting geochemical systems

AU Lee, Ming-Kuo; Bethke, Craig M.

Department of Geology, University of Illinois, Urbana, IL, 61801, USA CS

Am. J. Sci. (1996), 296(9), 965-988 CODEN: AJSCAP; ISSN: 0002-9599 SO

DT Journal

LA English

AB We present a numerical technique that predicts how the stable isotopes 2H, 13C, 18O, and 34S fractionate among solvent, aq. species, minerals, and gases over the course of a geochem. reaction process. Our model is based on mass balance techniques similar to those already presented in the literature but differs from previous techniques in that it allows minerals to be segregated from isotopic exchange instead of remaining in isotopic Such an approach allows us to simulate the fractionation of isotopes between rock and fluid resulting solely from mineral dissoln. and The technique was tested by modeling isotopic fractionation during several reaction processes, including (1) dolomitization of limestone by a migrating pore fluid, (2) diagenetic alteration of the Permian Lyons sandstone in the Denver basin, and (3) hydrothermal alteration of the Okanagan Batholith in southern British Columbia. The results of calcns. in which we segregate minerals from isotopic exchange compare well to isotopic trends obsd. in nature but differ markedly from calcns. that assume isotopic equil.

L12 ANSWER 14 OF 94 CA COPYRIGHT 2000 ACS

AN 125:203677 CA

- Using isotopic and molecular data to model landfill gas processes ΤI
- Bogner, J. E.; Sweeney, R. E.; Coleman, D.; Huitric, R.; Ririe, G. T. ΑU

CS Argonne National Laboratory, Argonne, IL, USA

SO Waste Manage. Res. (1996), 14(4), 367-376 CODEN: WMARD8; ISSN: 0734-242X

DT Journal

LA English

AB Using a large data set, a preliminary study was made to evaluate the usefulness of stable isotope ratios to improve the understanding of CH4 and CO2 generation in landfills. Included are ~130 landfill gas samples from across the USA, and 18 recent samples from: an Argonne Lab. study area in the Brea-Olinda Landfill, Orange County, California; and several Los

Angeles County landfills. The following isotope ratios were examd.:  $\delta$ 13C for CH4,  $\delta$ 13C for CO2, and  $\delta$ D for CH4. Using simple ratio plots supplemented by mass-balance calcns., these data showed promise to indicate the relative contributions of the 4 major C cycle processes in landfills: direct oxidn. of org. material to CO2; CH4 generation from fermn. (acetate cleavage); CH4 generation from CO2 redn.; and CH4 oxidn. to CO2 by methanotrophic bacteria. Both the CH4 generation and oxidn. reactions are central to explain the trends discussed. The data also suggested that direct oxidn. of org. matter in refuse may contribute to the obsd. isotopic ratios in some cases. Trends obsd. at the Brea-Olinda site were similar to trends using the large US database, suggesting that isotopic techniques may be useful to better constrain C cycle processes common to all landfill settings.

L12 ANSWER 18 OF 94 CA COPYRIGHT 2000 ACS

AN 125:66619 CA

TI Microbial utilization of estuarine dissolved organic carbon: a stable isotope tracer approach tested by mass balance

AU Hullar, Meredith A. J.; Fry, B.; Peterson, B. J.; Wright, R. T.

CS Org. Evolutionary Biol., Harvard Univ., Cambridge, MA, 02138, USA

SO Appl. Environ. Microbiol. (1996), 62(7), 2489-2493 CODEN: AEMIDF; ISSN: 0099-2240

LA English QR1.A6

- Plant natural stable isotope values were used to trace the fate of org. C that enters estuarine ecosystems. Expts. detd. the magnitude of δ13C changes of dissolved org. C (DOC) derived from tidal marsh vegetation during bacterial decompn. Bacteria were grown on DOC leached from estuarine Spartina alterniflora and Typhus angustifolia plants. In 4 expts., 25-80% of the initial C (2.6-9.1 mM org. C) was converted to bacterial biomass and CO2. Mass balance calcns. showed good recovery of total C and 13C at the end of these expts. (100% ± 14% total C; ± 1% δ13C). DOC δ13C values, bacterial biomass, and respired CO2 changed only slightly in the 4 expts. by av. values of -0.6, +1.4, and +0.5%, resp. These changes are small relative to the range of δ13C values represented by different org. C sources to estuaries. Thus, microbial δ13C values detd. in the field helped to identify the source of C assimilated by bacteria.
- LY2 ANSWER 21 OF 94 CA COPYRIGHT 2000 ACS

AN 124:155169 CA

TI Monitoring Crude Oil Mineralization in Salt Marshes: Use of Stable Carbon Isotope Ratios

AU Jackson, Andrew W.; Pardue, John H.; Araujo, Rochelle

- CS Department of Civil and Environmental Engineering, Louisiana State University, Baton Rouge, LA, 70803-7511, USA
- SO Environ. Sci. Technol. (1996), 30(4), 1139-44 CODEN: ESTHAG; ISSN: 0013-936X

LA English TD180.E5

In lab. microcosms using salt marsh soils and in field trials, it was possible to monitor and quantify crude oil mineralization by measuring changes in CO2 \$13C signatures and the rate of CO2 prodn. These values are easy to obtain and can be combined with simple isotope mass balance equations to det. the rate of mineralization from both the crude oil and indigenous carbon pool. Hydrocarbon degrdn. was confirmed by simultaneous decreases in alkane-, isoprenoid-, and PAH-hopane ratios. The pseudo-1st-order rate consts. of alkane degrdn. (0.087/day) and CO2 prodn. (0.082/day) from oil predicted by the \$13C signatures were statistically indistinguishable. The addn. of inorg. N and phosphate increased the rate of mineralization of crude oil in aerated microcosms but had no clear effect on in

situ studies. This procedure appears to offer a means of definitively quantifying crude oil mineralization in a sensitive, inexpensive, and simple manner in environments with appropriate background  $\delta$ 13C signatures.

- Lif2 ANSWER 24 OF 94 CA COPYRIGHT 2000 ACS
- AN 124:93073 CA
- TI Gas Chromatographic Isolation of Individual Compounds from Complex Matrixes for Radiocarbon Dating
- AU Eglinton, Timothy I.; Aluwihare, Lihini I.; Bauer, James E.; Druffel, Ellen R. M.; McNichol, Ann P.
- CS Department of Marine Chemistry and Geochemistry, Woods Hole Oceanographic Institution, Woods Hole, MA, 02543, USA
- SO Anal. Chem. (1996), 68(5), 904-12 CODEN: ANCHAM; ISSN: 0003-2700
- LA English
- This paper describes the application of a novel, practical approach for AΒ isolation of individual compds. from complex org. matrixes for natural abundance radiocarbon measurement. This is achieved through the use of automated preparative capillary gas chromatog. (PCGC) to sep. and recover sufficient quantities of individual target compds. for 14C anal. by accelerator mass spectrometry (AMS). This approach was developed and tested using a suite of samples (plant lipids, petroleums) whose ages spanned the 14C time scale and which contained a variety of compd. types (fatty acids, sterols, hydrocarbons). Comparison of individual compds. and bulk radiocarbon signatures for the isotopically homogeneous samples studied showed that  $\Delta$ 14C values generally agreed well ( $\pm$ 10%). Background contamination was assessed at each stage of the isolation procedure, and incomplete solvent removal prior to combustion was the only significant source of addnl. carbon. Isotope fractionation was addressed through compd.-specific stable carbon isotopic analyses. Fractionation of isotopes during isolation of individual compds. was minimal (<5 $\frac{3}{8}$  for  $\delta$ 13C), provided the entire peak was collected during PCGC. Trapping of partially coeluting peaks did cause errors, and these results highlight the importance of conducting stable carbon isotopic measurements of each trapped compd. in concert with AMS for reliable radiocarbon measurements. The addn. of carbon accompanying derivatization of functionalized compds. (e.g., fatty acids and sterols) prior to chromatog. sepn. represents a further source of potential error. This contribution can be removed using a simple isotopic mass balance approach. Based on these preliminary results, the PCGC-based approach holds promise for accurately detg. 14C ages on compds. specific to a given source within complex, heterogeneous samples.
- L12 ANSWER 27 OF 94 CA COPYRIGHT 2000 ACS
- AN 123:349619 CA
- TI Simple procedure for simultaneous recovery of dissolved inorganic and organic nitrogen in 15N-tracer experiments and improving the isotopic mass balance
- AU Slawyk, Gerd; Raimbault, Patrick
- CS Centre d'Oceanologie de Marseille, Faculte des Sciences de Luminy, Marseille, F-13288, Fr.
- SO Mar. Ecol.: Prog. Ser. (1995), Volume Date 1995, 124(1 to 3), 289-99 CODEN: MESEDT; ISSN: 0171-8630
- DT Journal
- LA English
- AB We developed a simple and reliable method which allows simultaneous isotope-ratio anal. of inorg. (DIN) and org. (DON) forms of N extd. from seawater. All forms of N under anal. are converted to ammonium, by diffusion with MgO, prior to collection on glass-fiber filters appropriate for mass spectrometric assay of 15N. Oxidized DIN forms (nitrate, nitrite)

are reduced to ammonium in the presence of Devarda alloy. Conversion of DON to ammonium is performed by wet oxidn. using K persulfate and subsequent redn. of the nitrate formed. Recovery tests, for total N and 15N content, showed that this procedure is suitable for application in DI15Nisotope diln. expts. and DON-release studies. Recovery of total N from DIN and DON was nearly complete (94-97 %). The variability in the exptl. detn. of 15N abundance was <2% and <4% for DIN and DON, resp. We used the method to balance the 15N budget in nitrate and ammonium uptake expts. conducted in an oligotrophic area (tropical North Atlantic) by including, in addn. to the substrate (DIN) and biomass (PON) pool, the DON pool. However, the use of glass-fiber filters (GF/F) for the collection of particulate matter produced a significant artifact. While inclusion of this combined pool led virtually to a complete accounting for the 15N label (99%) in all samples for nitrate uptake and in those for ammonium uptake incubated for <8 h, no mass balance was achieved during ammonium uptake lasting 10-24 h. suggest that the 15N that was still missing (13%) resulted mainly from bottle containment effects such as ammonium-ion adsorption and/or PON adherence onto incubation bottle walls. Transfer of 15N label to the combined pool (nitrate expt.) and to the DON and GF/F-related PON pools (ammonium expt.) represented up to 41, 38, and 20% of the total 15N taken up as DIN, resp., and depended strongly upon the length of incubation. Failure to take these pathways of the missing 15N into account during traditional 15N uptake expts. involves risk of substantially underestimating new and regenerated prodn., at least in oligotrophic areas. The latter has considerable significance in the design of future 15N tracer methodologies.

L√2 ANSWER 38 OF 94 CA COPYRIGHT 2000 ACS

AN 121:220675 CA

TI Derivatization of organic compounds prior to gas chromatographiccombustion-isotope ratio mass spectrometric analysis: identification of isotope fractionation processes

AU Rieley, Gareth

CS School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK

SO Analyst (Cambridge, U. K.) (1994), 119(5), 915-19 CODEN: ANALAO; ISSN: 0003-2654

LA English

An examn. of the practice of derivatizing org. compds. such as fatty acids, AΒ sterols and amino acids in relation to subsequent anal. via gas chromatog.combustion-isotope ratio mass spectrometry is presented. Fractionation processes, such as kinetic isotope effects, which cause a deviation in the measured stable C isotope ratios ( $\delta$ -values) of derivatized compds. from simple mass balance considerations are examd. Particular attention is paid to reactions that proceed by the cleavage of a C-contg. bond and reactions that probably have kinetic isotope effects assocd. with them, such as acetylation and diazotization. Isotope fractionation processes other than those which are kinetic based are also discussed, as is the addnl. imprecision of the calcn. of the  $\delta$ -values of sample compds. inherent when Failure to take this imprecision into account when deriv. C is added. comparing  $\delta$ -values could lead to erroneous conclusions with respect to the magnitude of kinetic isotope effects caused by deriv. reactions.

- L12 ANSWER 40 OF 94 CA COPYRIGHT 2000 ACS
- AN 121:113 CA
- TI Performance of human mass balance/metabolite identification studies using stable isotope (13C, 15N) labeling and continuous-flow isotope-ratio mass spectrometry as an alternative to radioactive labeling methods
- AU Browne, Thomas R.; Szabo, George K.; Ajami, Alfred; Wagner, David

CS Sch. Med., Boston Univ., Boston, MA, USA

SO J. Clin. Pharmacol. (1993), 33(3), 246-52 CODEN: JCPCBR; ISSN: 0091-2700

DT Journal

LA English

Stable isotope labeling in therapeutic and subtherapeutic quantities of drug (15N213C-phenobarbital) can be quantitated in biol. matrixes (urine) and high performance liq. chromatog. (HPLC) peaks from urine using continuous-flow isotope-ratio mass spectrometry (CF-IRMS). Std. curves for 15N213C-phenobarbital were reproducible and linear (R2 > 0.985) over the ranges of 3-100  $\mu \text{g/mL}$  for whole urine (15N2 or 13C labeling) and 0.1-8.0  $\mu \text{g/mL}$  for HPLC peaks derived from urine (15N2 labeling). The lower limit of quantitation values for urine drug concn. was 0.46-2.62  $\mu \text{g/mL}$  in whole urine and 0.10-0.70  $\mu \text{g/mL}$  in HPLC peaks. Validation samples quantitated with these std. curves yielded close to expected values. These data suggest stable isotope labeling and CF-IRMS may be used as an alternative to 14C labeling and radioactivity counting methods in mass balance/metabolite identification and other biomedical studies.

L12 ANSWER 41 OF 94 CA COPYRIGHT 2000 ACS

AN 120:330445 CA

TI NETPATH: An interactive code for interpreting NET geochemical reactions from chemical and isotopic data along a flow PATH

AU Plummer, L. Niel; Prestemon, Eric C.; Parkhurst, David L.

CS US Geol. Surv., Reston, VA, USA

SO Water-Rock Interact., Proc. Int. Symp., 7th (1992), Volume 1 239-42. Editor(s): Kharaka, Yousif K.; Maest, Ann S. Publisher: Balkema, Rotterdam, Neth. CODEN: 58KXA2

DT Conference

LA English

NETPATH is an interactive Fortran 77 computer program used to interpret net geochem. mass-balance reactions between initial and final waters along a hydrol flow path. The program uses chem. and isotopic data for waters from a hydrochem. system. The processes of dissoln., pptn., ion exchange, oxidn./redn., degrdn. of org. compds., incongruent reaction, gas exchange, mixing, evapn., diln., isotope fractionation, and isotope exchange can be considered. Geochem. mass-balance reaction models are examd. between selected evolutionary waters for every possible combination of the plausible phases that account for the compn. of a selected set of chem. and isotopic constraints in the system. The NETPATH software includes a database program, DB, for storing and editing chem. and isotopic data for use in NETPATH.

ANSWER 57 OF 94 CA COPYRIGHT 2000 ACS

AN 115:197428 CA

TI Determination of the concentration and stable isotopic composition of nonexchangeable hydrogen in organic matter

AU Schimmelmann, Arndt

CS Scripps Inst. Oceanogr., Univ. California, La Jolla, CA, 92093-0215, USA

SO Anal. Chem. (1991), 63(21), 2456-9 CODEN: ANCHAM; ISSN: 0003-2700

LA English

L1**V** 

The hydrogen state isotope ratio of org. matter contg. hydrogen that is not solely conservative, nonexchangeable, carbon-bond hydrogen depends on sample prepn., because org. hydrogen bound to oxygen and nitrogen may exchange isotopically with ambient-water hydrogen. The method described here permits the detn. of the concn. and stable isotopic compn. of the nonexchangeable hydrogen in complex org. matter, such as geochems. and biol. and archaeol. org. materials. Aliquots of org. substrates were independently equilibrated with water vapors of different hydrogen isotopic

compns., followed by detns. of the bulk D/H ratios. Mass-balance calcns. permit eliminating or minimizing the interference of exchangeable hydrogen. The precision of the calcd. stable isotope ratio of nonexchangeable hydrogen can be better than ±3 per mil, depending on the precision of the measured values for bulk hydrogen. The accuracy of D/H ratios of nonexchangeable hydrogen was improved over that of previously available methods, as shown for cellulose/cellulose nitrate.

ANSWER 63 OF 94 CA COPYRIGHT 2000 ACS

114:125595 CA

Stable carbon isotope analysis of products from coal/tar sand bitumen coprocessing

Keogh, Robert A.; Hardy, Rita H.; Davis, Burtron H. ΑU

Cent. Appl. Energy Res., Univ. Kentucky, Lexington, KY, 40511-8433, USA CS SO

Energy Fuels (1991), 5(2), 322-7 CODEN: ENFUEM; ISSN: 0887-0624

TP315.E518 LΑ mainmic English

A western Kentucky No. 9 coal and tar-sand bitumen were catalytically AB coprocessed by using the CAER 1/8 ton/day pilot plant facility. feedstocks and products were extensively characterized. The  $\sigma$ 13C ratios of the fractions were utilized to det. quant. the contribution of the coal and tar sand bitumen to the product slate. The coal contribution to the coprocessing product slate was greatest in the heavy distillate and resid Processing caused fractionation of the C isotopes which must be accounted for in the mass balance calcns. Fractionation of the C isotopes was greatest in the product gases and the naphtha fraction.

ANSWER 66 OF 94 CA COPYRIGHT 2000 ACS

ΑN 114:61125

Stable carbon isotope analysis of amino acid enantiomers by conventional TI isotope ratio mass spectrometry and combined gas chromatography/isotope ratio mass spectrometry

Silfer, J. A.; Engel, M. H.; Macko, S. A.; Jumeau, E. J. ΑU

CS Sch. Geol. Geophys., Univ. Oklahoma, Norman, OK, 73019, USA

SO CODEN: ANCHAM; ISSN: 0003-2700 Anal. Chem. (1991), 63(4), 370-4

LAEnglish

L102

AB

The application of a combined gas chromatog./isotope ratio mass spectrometry (GC/IRMS) method for stable C isotope anal. of amino acid enantiomers is presented. This method eliminates the numerous preparative steps integral to the isolation of amino acids and amino acid enantiomers from protein hydrolyzates that precede  $\delta$ 13C anal. by conventional isotope ratio mass spectrometry. Unlike hydrocarbons, amino acids require derivatization prior to GC/IRMS anal. Replicate  $\delta$ 13C analyses of trifluoroacetyl (TFA) iso-Pr ester derivs. of 22 amino acids by IRMS revealed that the derivatization process is reproducible, with an av. error (1 std. deviation) of  $0.10\% \pm 0.09\%$ . The av. anal. error for anal. of amino acid derivs. by GC/IRMS was 0.26%  $\pm$  0.09%. In general, abs. differences between IRMS and GC/IRMS analyses were <0.5%. The derivatization process introduces a distinct, reproducible isotopic fractionation that is const. for each amino acid type. The obsd. fractionations preclude direct calcn. of underivatized amino acid  $\delta$ 13C values from their resp. TFA iso-Pr ester 813C compns. through mass balance relation. Derivatization of amino acid stds. of known stable C isotope compn. in conjunction with natural samples, however, permits computation of the original, underivatized amino acid  $\delta$ 13C values through use of an empirical correction for the C introduced during the derivatization process.

CA COPYRIGHT 2000 ACS L12 ANSWER 73 OF 94 AN109:196761 CA

- TI The fate of trace metals in suspended matter in a mangrove creek during a tidal cycle
- AU Lacerda, L. D.; Martinelli, L. A.; Rezende, C. E.; Mozeto, A. A.; Ovalle, A. R. C.; Victoria, R. L.; Silva, C. A. R.; Nogueira, F. B.
- CS Dep. Geoquim., Univ. Fed. Flaminense, Niteroi, 24210, Brazil
- SO Sci. Total Environ. (1988), 75(2-3), 169-80 CODEN: STENDL; ISSN: 0048-9697
- DT Journal
- LA English
- The variation of heavy metal content in suspended matter (SM) during tidal AΒ cycles in a mangrove creek is described. The stable isotope of C was used as a tracer for sources of SM to the system. During tidal cycles, 3 patterns of metal variability were found. The 1st, represented by Fe, showed an irregular and small variability throughout the cycle; the 2nd represented by Mn, exhibited a sharp increase in concn. during the rising tide, coincident with the greatest variation of pH and Eh. The 3rd pattern, including Cu, Cd, Pb, Ni, Cr, and Zn, showed max. concn. at the peak of the high tide, coincident with a shift in SM source. The stable isotope of C indicated that, during low tides, most of the org. C exported originated from mangrove plant detritus, while during the high tides org. C imported by the system was almost totally of marine origin. This shift of SM source is the principal parameter controlling metal fluxes through the system. Changes in water pH and Eh and in Mg pptn. can also serve as a secondary control. Although the results strongly suggest that the metallic load of marine SM is being immobilized by the mangrove environment, mass balance studies are necessary to show whether a net accumulation of metals is actually occurring.
- L12 ANSWER 78 OF 94 CA COPYRIGHT 2000 ACS
- AN 106:216709 CA
- TI Use of stable sulfur isotopes to monitor directly the behavior of sulfur in coal during thermal desulfurization
- AU Liu, C. L.; Hackley, K. C.; Coleman, D. D.
- CS Illinois State Geol. Surv., Champaign, IL, 61820, USA
- SO Fuel (1987), 66(5), 683-7 CODEN: FUELAC; ISSN: 0016-2361
- LA English TP315.F85 evolur
- A method was developed by using stable S isotope analyses to monitor the AΒ behavior of S forms in a coal during thermal desulfurization. method, the natural stable isotopic compn. of the pyritic and org. S in coal is used as a tracer to follow their mobility during the desulfurization process. This tracer method is based on the fact that the isotopic compns. of pyritic and org. S are significantly different in some Isotopic results of pyrolysis expts. at 350-750° indicate that the S released with the volatiles is predominantly org. S. The pyritic S is evolved in significant quantities only when pyrolysis temps. are >500°. The presence of pyrite has no effect on the amt. of org. S evolved during The chem. and isotopic mass balances achieved from 3 different pyrolysis. samples of the Herrin (No. 6) coal of the Illinois Basin demonstrate that this stable isotope tracer method is quant. The main disadvantage of this tracing technique is that not all coals contain isotopically distinct org. and pyritic S.
- L12 ANSWER 85 OF 94 CA COPYRIGHT 2000 ACS
- AN 100:44818 CA
- TI Stereochemical composition of propranolol metabolites in the dog using stable isotope-labeled pseudoracemates
- AU Walle, Thomas; Wilson, Michael J.; Walle, U. Kristina; Bai, Stephen A.
- CS Dep. Pharmacol., Med. Univ. South Carolina, Charleston, SC, 29425, USA
- SO Drug Metab. Dispos. (1983), 11(6), 544-9 CODEN: DMDSAI; ISSN: 0090-9556

DT Journal LA English

The stereochem. compn. of racemic propranolol [13013-17-7] and its AΒ metabolites was detd. in the urine of dogs after single 160-mg oral doses of stable isotope-labeled pseudoracemates of propranolol. All major metabolites, accounting for 84% of the dose excreted in urine, were isolated by solvent extn. or high-performance liq. chromatog., glucuronic acid conjugates after enzymic hydrolysis, and analyzed by gas chromatog.-mass spectrometry after chem. derivatization. Of the 3 primary metabolic pathways, glucuronidation of the parent drug, about 16% of the dose recovered in urine, was highly selective for (-)-propranolol [4199-09-1], (-)/(+)-enantiomer [5051-22-9] ratio 3.5. In contrast, all of the side-chain oxidn. metabolites, about 30% of the dose, were mainly derived from (+)-propranolol, (-)/(+)-enantiomer ratio ranging from 0.35 to Ring oxidn., involved in the metab. of the remainder of the dose studied, about 38%, was, however, also found to be selective for (-)-propranolol, with the greatest selectivity obsd. in 4'-hydroxypropranolol [69499-28-1], (-) - [76792-96-6]/(+) -enantiomer [76792-97-7] There was an excellent mass balance for the enantiomers of the metabolites studied, i.e. the total (-)/(+)-enantiomer ratio was close to unity. The higher oral bioavailability of (+)-propranolol in the dog, well reflected in the stereochem. compn. of unchanged propranolol in urine, is suggested to be due to stereoselective presystemic hepatic removal of (-)-propranolol by glucuronidation and ring oxidn.

ANSWER 92 OF 94 CA COPYRIGHT 2000 ACS

AN 82:174715 CA

L1X

TI Trace element mass balance around a coal-fired steam plant

AU Bolton, N. E.; Carter, J. A.; Emery, J. F.; Feldman, C.; Fulkerson, W.; Hulett, L. D.; Lyon, W. S.

CS Oak Ridge Natl. Lab., Oak Ridge, Tenn., USA

SO Am. Chem. Soc., Div. Fuel Chem., Prepr. (1973), 18(4), 114-23 CODEN: ACFPAI

LA English TP315.A5 mainmic

In a collaborative effort between Oak Ridge National Laboratory and the AΒ Tennessee Valley Authority, mass balance measurements for some 41 elements were made around the Thomas A. Allen Steam Plant in Memphis, Tennessee. For 1 of the 3 independent cyclone boilers at the plant, the concn. and flow rates of each element were detd. for the coal, the slag tank effluent, the fly ash in the precipitator inlet and outlet (collected isokinetically at a representative series of duct locations detd. by the gas flow profiles), and fly ash in the stack gases (collected isokinetically at the 268 ft level). Measurements by neutron activation anal., spark source mass spectroscopy (with isotope diln. for some elements), and atomic adsorption spectroscopy yielded an approx. balance (closure to ~30%) for many Exceptions were those elements forming volatile compds. such as elements. For most elements in the fly ash the newly installed electrostatic precipitators were extremely efficient. Se is an exception.

=> log y STN INTERNATIONAL LOGOFF AT 16:52:32 ON 15 FEB 2000 L1

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(FILE 'HOME' ENTERED AT 12:09:00 ON 15 FEB 2000) FILE 'CA' ENTERED AT 12:09:07 ON 15 FEB 2000 E PICKUP J/AU 2 S E3-13 AND 1976/PY E KORZEKWA K/AU 15 S E3-8 AND TRAGER W?/AU 1 S L2 AND MASS/SO 1 S LEE W?/AU AND WHITING J?/AU AND FYMAT A?/AU 9 S LEE W?/AU AND 1989/PY AND BIOL?/SO 3 S L5 AND MASS 10238 S STABLE(2A) ISOTOP? 1298 S L7 AND (ALGOR? OR EQUATION OR CALCULAT?) 328 S L8 AND (ERROR OR CORRECT? OR CONVERT? OR CONVERSION OR OXIDIZ? OR REDUC? OR OXIDAT?) 17 S L8 AND (SPIKE? OR SPIKING) 74 S L7 AND (SAMPLE OR SAMPLING OR ION?) (4A) (INTEGRIT? OR QUALITY OR CONVER? OR OXIDAT? OR REDOX OR REDUC? OR OXIDIZ?) 30 S L7 AND SPECIAT? 18 S L7 AND DECONVOL? 375 S L9-13 NOT PY>1997 347 S L14 NOT (BOREHOLE OR NOBLE GAS OR VIVO OR INSULIN OR PETROLOG?) 28 S L14 NOT L15 6 S L16 AND ENRICH? 105 S L10-13 AND L15 242 S L15 NOT L18 37 S L19 AND ((TURNOVER OR REDUCTION OR INCORPORAT? OR DUAL OR OXIDAT?)/TI OR VARIABILITY OR SPECIE (1A) SPECIFIC OR MATHEMAT?) 153 S L1, L3-4, L6, L17-18, L20 => d 121 bib, ab 1-153 ANSWER 4 OF 153 CA COPYRIGHT 2000 ACS 127:306852 CA Stable isotope labels as a tool to determine the iron absorption by Peruvian school children from a breakfast meal Walczyk, Thomas; Davidsson, Lena; Zavaleta, Nelly; Hurrell, Richard F. Labor Humanernahrung, Eidgenossische Technische Hochschule Zurich, Rueschlikon, CH-8003, Switz. Fresenius' J. Anal. Chem. (1997), 359(4-5), 445-449 CODEN: FJACES; ISSN: 0937-0633 Journal English Fractional Fe absorption from a breakfast meal was detd. in Peruvian

- DTLA
- AB children employing stable Fe isotopes as labels. Fe isotopic anal. was performed by the recently developed neg. thermal ionization technique for high-precision Fe isotope ratio measurements using FeF4- ions. By increasing the ascorbic acid content of the std. breakfast meal as served within the Peruvian school-breakfast program from 27 mg to 70 mg, it was possible to increase the geometric mean fractional Fe absorption significantly from 5.1% (range 1.6-13.5%) to 8.2% (range 3.1-25.8%). Fractional Fe absorption was calcd. according to isotope diln. principles and by considering the non-monoisotopic character of the used spikes.
- L21 ANSWER 5 OF 153 CA COPYRIGHT 2000 ACS
- AN127:304820 CA
- TIApplications of mass spectrometry in the trace element analysis of

biological materials

- AU Moens, Luc
- CS Laboratory Analytical Chemistry, University Ghent, Ghent, B-9000, Belg.
- SO Fresenius' J. Anal. Chem. (1997), 359(4-5), 309-316 CODEN: FJACES; ISSN: 0937-0633
- DT Journal; General Review
- LA English
- AP A review with 32 refs. is given. The importance of mass spectrometry for the anal. of biol. material is illustrated by reviewing the different mass spectrometric methods applied and describing some typical applications published recently. Though at. absorption spectrometry is used in the majority of analyses of biol. material, most mass spectrometric methods have been used to some extent for trace element detn. in biomedical research. The relative importance of the different methods is estd. by reviewing recent research papers. It is striking that esp. inductively coupled plasma mass spectrometry is increasingly being applied, partly because the method can be used online after chromatog. sepn., in speciation studies. Mass spectrometric methods prove to offer unique possibilities in stable isotope tracer studies and for this purpose also exptl. demanding methods such as thermal ionization mass spectrometry and accelerator mass spectrometry are frequently used.

## L21 ANSWER 8 OF 153 CA COPYRIGHT 2000 ACS

- AN 127:75317 CA
- TI Determination of artifactual formation of monomethylmercury (MeHg+) in environmental samples using stable Hg2+ isotopes with ICP-MS detection. Calculation of contents applying species specific isotope addition
- AU Hintelmann, H.; Falter, R.; Ilgen, G.; Evans, R. D.
- CS Environmental Science Center, Trent Univ., Peterborough, ON, K9J 7B8, Can.
- SO Fresenius' J. Anal. Chem. (1997), 358(3), 363-370 CODEN: FJACES; ISSN: 0937-0633
- DT Journal
- LA English
- AB Various extn. techniques, such as distn. and acid and alk. extn., were tested with regard to their potential to form a MeHg artifact from inorg. Hg during sample prepn. Hg2+ was added to different ref. materials in the form of enriched stable tracers and the formation of new MeHq from that tracer was analyzed by HPLC/inductively coupled plasma (ICP)-mass spectrometry (MS) and gas chromatog. (GC)/ICP-MS. Both techniques gave comparable results. In particular, the distn. technique was prone to The resulting overestimation of MeHg in sediments was artifact formation. as high as 80%. Artifact formation in hair, liver, and algae samples was less significant, though still observable. Fish muscle tissue showed no artifact formation upon distn., but some of the inorg. tracer was converted to MeHg during alk. extn. Acid extn. of sediments resulted in low artifact formation rates. Fractionated measurements of sediment distillates revealed high MeHg formation rates towards the end of the distn. process when acid concns. in the soln. are highest. A technique for correction of the measured apparent MeHg content applying species-specific isotope addn. (SSIA) is proposed and the calcn. scheme is presented.
- L21 ANSWER 17 OF 153 CA COPYRIGHT 2000 ACS
- AN 125:80831 CA
- TI Analytical plasma source mass spectrometry in biomedical research
- AU Barnes, Ramon M.
- CS Lederle Graduate Research Center, University Massachusetts, Amherst, MA, 01003-4510, USA
- SO Fresenius' J. Anal. Chem. (1996), 355(5-6, XXIX Colloquium Spectroscopicum

Internationale, 1995), 433-441 CODEN: FJACES; ISSN: 0937-0633

DT Journal; General Review

LA English

A review with 100 refs. The features of inductively coupled plasma-mass spectrometry (ICP-MS) that make it unique also make possible applications in biol. chem. and biomedical research that would be otherwise difficult or impossible. High sensitivity, characterized spectral interferences, rapid mass scanning and individual isotope measurements are now combined with sophisticated sample prepn., sepns., or stable isotope addns. to achieve rapid semi-quant. anal., element speciation, and high accuracy. The semi-quant. anal. of various materials, the sepn. and detection of macromols. in blood and other tissues, and tracking of stable isotopes added either purposely or inadvertently to children are important applications of ICP-MS. Current functional limitations and obstacles and potential development areas also are examd.

L21 ANSWER 19 OF 153 CA COPYRIGHT 2000 ACS

AN 124:336995 CA

TI Simultaneous speciation of endogenous and exogenous elements by HPLC/ICP-MS with enriched stable isotopes

AU Suzuki, Kazuo T.

CS Faculty Pharmaceutical Sciences, Chiba University, Chiba, 263, Japan

SO Tohoku J. Exp. Med. (1996), 178(1), 27-35 CODEN: TJEMAO; ISSN: 0040-8727

DT Journal

LA English

HPLC/inductively coupled argon plasma-mass spectrometry (ICP-MS) was AB introduced to investigate the distributions of Se in biol. fluids. method was to det. both the natural abundance of Se and an enriched stable isotope of Se used as a tracer. The distributions of Se in plasma and in urine specimens were detd. in Wistar rats on various Se diets with and without an i.v. injection of 82Se-selenite. Although the distribution of natural abundance Se (endogenous Se) in the plasma was affected little by the nutritional status of Se, that in the urine gave a Se peak depending on the nutritional status of Se, and the peak was identified as methylselenol. When 82Se-selenite was injected in excess into rats given three different Se diets (Se-deficient, Se-adequate, Se-excessive), three Se peaks occurred in the HPLC chromatogram of the urine samples, corresponding to selenite, methylselenol and trimethylselenonium ion in the order of elution, and the intensities of the tracer peaks reflected the nutritional status. HPLC/ICP-MS method is a powerful anal. tool for specifying Se-contg. biol. constituents, both natural abundance and enriched stable isotopes. Methylselenol in urine is proposed to be a sensitive and Se-specific biol. indicator for diagnosing the nutritional status of Se. Furthermore, it was shown that an enriched stable isotope such as 82Se-selenite was shown to be used for the same purpose, and that 82Se-methylselenol and 82Setrimethylselenonium ion in urine were more sensitive indicators of the Se status of the rats.

## ANSWER 20 OF 153 CA COPYRIGHT 2000 ACS

AN 124:311682 CA

TI Gas chromatography-mass spectrometry analysis of vitamin E and its oxidation products

AU Liebler, Daniel C.; Burr, Jeanne A.; Philips, Leslie; Ham, Amy J. L.

CS Dep. Pharmacol. Toxicol., Coll. Pharm., Univ. Arizona, Tucson, AZ, 85721, USA

SO Anal. Biochem. (1996), 236(1), 27-34 CODEN: ANBCA2; ISSN: 0003-2697

DT Journal

LA English

To facilitate studies of vitamin E ( $\alpha$ -tocopherol) antioxidant actions in AΒ tissues, we have developed a stable isotope diln. capillary gas chromatoq.mass spectrometry assay for  $\alpha$ -tocopherol and its three principal oxidn. products,  $\alpha$ -tocopherolquinone, 5,6-epoxy- $\alpha$ -tocopherolquinone, 2,3-epoxy- $\alpha$ tocopherolquinone, and for  $\alpha$ -tocopherolhydroquinone, a redn. product of  $\alpha$ tocopherolquinone. Deuterium-labeled internal stds.  $5,7-[2H3-methyl]-\alpha$ tocopherol, 2,6-[2H3-methyl]- $\alpha$ -tocopherolquinone, 2,6-[2H3-methyl]-5,6epoxy- $\alpha$ -tocopherolquinone, 2,6-[2H3-methyl]-2,3-epoxy- $\alpha$ -tocopherolquinone, and 2-[2H3-methyl]- $\alpha$ -tocopherolhydroquinone are added to cell or tissue The products then are extd. and converted to O-trimethylsilyl Products are analyzed by capillary gas chromatog. with on-column injection and detected by selected ion monitoring of characteristic fragment ions in electron ionization mode. Std. curves were linear from 25 fmol to 2 pmol for products and from 25 fmol to 4 pmol for  $\alpha$ -tocopherol. The use of 2H6- and 2H3-internal stds. for  $\alpha$ -tocopherolquinone and  $\alpha$ tocopherolhydroquinone permits simultaneous anal. of both products despite α-Tocopherol oxidized possible redox interconversion during sample workup. in microsomes treated with azo-bis(amidinopropane HCl) was quant. accounted for as the epoxyguinones,  $\alpha$ -tocopherolquinone, and  $\alpha$ -tocopherolhydro-However, over half of the oxidn. products were present in microsomes as acid-labile tocopherone precursors. This method permits comprehensive assessment of vitamin E status in tissues and quant. studies of vitamin E antioxidant actions and turnover.

L21 ANSWER 29 OF 153 CA COPYRIGHT 2000 ACS

AN 123:305549 CA

Measurement of mercury methylation in sediments by using enriched stable mercury isotopes combined with methylmercury determination by gas chromatography-inductively coupled plasma mass spectrometry

AU Hintelmann, Holger; Evans, R. Douglas; Villeneuve, Janice Y.

CS Environ. Sci. Cent., Trent Univ., Peterborough, ON, K9J 7B8, Can.

SO J. Anal. At. Spectrom. (1995), 10(9), 619-24 CODEN: JASPE2; ISSN: 0267-9477

DT Journal

LA English

AΒ

A novel technique for the calcn. of Hg methylation rates in sediments by using enriched stable Hg isotopes is described. The method takes advantages of the ability of an inductively coupled plasma mass spectrometry (ICP-MS) instrument to measure individual isotopes. instrument was used as a detector for the detn. of methylmercury compds. after sepn. by gas chromatog. (GC). MeHg+ was isolated from sediments by distn., converted to methylethylmercury by Na tetraethylborate and analyzed after purge-and-trap precollection on a Tenax adsorber and thermodesorption onto the GC column. Detection limits are ≈1 pg (as Hg) abs. or 0.02 ng g-1 The precision was ≈4% relative std. deviation when 250 pg of dry sediment. methylmercury were processed. The accuracy of the GC-ICP-MS technique was demonstrated by anal. of an International At. Energy Agency certified ref. material (IAEA CRM 356) Harbor Sediment, giving a concn. of 5.40  $\pm$  0.40 ng g-1, compared with the certified value of  $5.47 \pm 0.38$  ng g-1. methylation was studied by spiking sediments with stable enriched Hg isotopes at in situ Hg concns. not perturbing the system. More than 3% of the Hg added to a lake sediment was methylated during a 21 d incubation period. Isotope ratios of total Hg differed significantly from isotope ratios of methylmercury at the end of the expt., suggesting that the system was still not in equil. after 21 d.

ANSWER 46 OF 153 CA COPYRIGHT 2000 ACS

AN 121:152731 CA

TI Assay of malondialdehyde in biological fluids by gas chromatography-mass

spectrometry

Yeo, Helen C.; Helbock, Harold J.; Chyu, Daniel W.; Ames, Bruce N. AU

Div. Biochem. Mol. Biol., Univ. California, Berkeley, CA, 94720, USA

Anal. Biochem. (1994), 220(2), 391-6 CODEN: ANBCA2; ISSN: 0003-2697 SO

DT Journal

CS

LA English

Malondialdehyde (MDA) is assayed in femtomole quantities in biol. samples AΒ by gas chromatog.-mass spectrometry (GC-MS). The MDA trapped in protein as a Schiff base is released by H2SO4, the protein pptd. using Na2WO4, and the MDA derivatized with pentafluorophenylhydrazine to form the stable adduct, N-pentafluorophenylpyrazole. Neg. chem. ionization (NCI) capability allows the sensitive detection of this MDA adduct in biol. samples at a level of 5 nM on-column. A stable-isotope -labeled MDA, [2H2]MDA, was used as an internal std. for quantitation. MDA recovery from plasma was 76%. assay provides two forms of confirmation of the analyte, retention time and mass ion, thus minimizing error due to interfering compds. The commonly used thiobarbituric acid assay for MDA overestimates the MDA levels by over 10-fold, possibly resulting from cross-reactivity with other aldehydes and artifactual oxidn. due to 100° temp. conditions. In the authors' assay, all steps were performed at room temp. thereby suppressing artifactual oxidn. of the sample. The authors have successfully applied this assay to biol. samples including plasma, tissue homogenates, and sperm.

ANSWER 47 OF 153 CA COPYRIGHT 2000 ACS

121:103424 CA ΑŃ

ΤI Method for computing the oxidation of two carbon 13-substrates ingested simultaneously during exercise

Peronnet, Francois; Adopo, Eudoxie; Massicotte, Denis; Brisson, Guy R.; ΑU Hillaire-Marcel, Claude

CS Inst. Nat. Rech. Sci.-Sante, Univ. Montre., Montreal, PQ, H3C 3J7, Can. SO

J. Appl. Physiol. (1993), 75(3), 1419-22 CODEN: JAPHEV; ISSN: 8750-7587

DTJournal

Грг

AΒ

LA English

This study presents a method for computing the resp. amts. of two simultaneously ingested exogenous substrates (A and B) that are oxidized during a period of prolonged exercise by use of 13C labeling. is based on the observation that the total vol. of 13CO2 produced (V13CO2tot) is the sum of (1) V13CO2 arising from the oxidn. of endogenous substrates (V13CO2 endo), (2) V13CO2 arising from the oxidn. of substrate A (V13CO2A), and (3) V13CO2 arising from the oxidn. of substrate B (V13CO2B). The equation, V13CO2 tot = V13CO2 endo + V13CO2A + V13CO2B, with three unknowns, can be solved from the results of three expts. conducted under the same conditions but with at least two values for the isotopic compn. of This method has been used on five healthy male subjects to compute the amts. of glucose and fructose oxidized when a mixt. of 15 q of glucose and 15 g of fructose is ingested (in 300 mL of water) over 60 min of cycle ergometer exercise at 65% of maximal O2 uptake. Results from three expts. indicated that 9.8  $\pm$  3.1 and 5.7  $\pm$  2.1 g of glucose and fructose, resp., were oxidized. The total amt. of exogenous carbohydrates oxidized (15.5  $\pm$  4.3 g) is in agreement with the oxidn. rates of exogenous glucose computed in similar conditions when 30 g of glucose were ingested (13 g; Peronnet et al. Med. Sci. Sports Exercise 25: 297-302, 1993). difference between the oxidn. rates of exogenous glucose and fructose is also in line with data from the literature.

ANSWER 51 OF 153 CA COPYRIGHT 2000 ACS L21

119:220967 AN

The measurement of exchangeable pools of zinc using the stable isotope 70Zn TI

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SO Br. J. Nutr. (1993), 70(1), 221-34 CODEN: BJNUAV; ISSN: 0007-1145

DT Journal

LA English

AB

The present study was designed to assess the feasibility of using small doses of a stable isotope of Zn to follow plasma kinetics over a 10-day period and, hence, make deductions about In turnover and body pool sizes. At the beginning of the 10-day metabolic balance, two adults, consuming their habitual diet, were given an i.v. injection of 70Zn. There was a fourfold difference in the administered dose between the two subjects (0.445 and 2.078 mg). Blood samples were taken at regular intervals and plasma enrichment with 70Zn measured by thermal ionization mass spectrometry. Urine and feces were collected and analyzed for Zn and 70Zn. Kinetic anal. of plasma 70Zn decay by several different methods was undertaken. It was apparent from both deconvolution anal. of the shortterm (0-90 min) decay data and four-compartment modeling of the longer-term (0-24 h) data that isotopic Zn very rapidly equilibrates with the plasma Zn and with a rapidly exchanging non-plasma pool, probably located within the This latter pool appears to contain less than 10 mg Zn and the peak of isotope enrichment occurs at about 20 min post injection. The later decay of plasma Zn enrichment appears to be dictated by exchange with a much larger pool of approx. size 350 mg.

ANSWER 68 OF 153 CA COPYRIGHT 2000 ACS

AN 116:234380 CA

Utilization of two different chemical forms of selenium during lactation using stable isotope tracers: an example of speciation in nutrition

AU Moser-Veillon, Phylis B.; Mangels, A. Reed; Patterson, Kristine Y.;

Veillon, Claude

CS Dep. Hum. Nutr. Food Syst., Univ. Maryland, College Park, MD, 20742, USA SO Analyst (London) (1992), 117(3), 559-62 CODEN: ANALAO; ISSN: 0003-2654

DT Journal LA English

AB

L**2**1

As an example of speciation questions addressed by nutritionists, a study is described that simultaneously evaluated utilization (absorption, retention and appearance in milk and blood) of two different chem. forms of selenium (selenite and selenomethionine) in lactating, non-lactating and never pregnant women using stable isotope tracers. All three groups of women had similar selenium had similar selenium status at the start of the Significantly more selenonmethione than from selenite was absorbed and appeared in the plasma in all groups. Milk contained more selenium from apparently absorbed selenomethionine than from selenite. All groups retained significantly more selenium from selenomethionine than from selenite; lactating women retained more selenium from selenite than did the other two groups, suggesting that milk losses may be partially compensated by enhanced retention of dietary selenium as selinite. Absorption and retention of selenium from selenomethionine in lactating women did not appear to be different from the other groups. The different chem. forms of selenium are metabolized differently among different physol. groups of

ANSWER 84 OF 153 CA COPYRIGHT 2000 ACS

AN 111:111867 CA

TI Analysis of mass isotopomer data

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SO J. Biol. Chem. (1989), 264(22), 13002-4 CODEN: JBCHA3; ISSN: 0021-9258

DT Journal

LA English

AB For use in metabolic studies with stable isotope indicators, an algorithm for background correction in isotopomer anal., is discussed and equations are derived for the parameters of the Krebs cycle metabolic model.

LY 1 ANSWER 89 OF 153 CA COPYRIGHT 2000 ACS

AN 111:53633 CA

TI Isotopic determination of selenium in biological materials with inductively coupled plasma mass spectrometry

AU Ting, Bill T. G.; Mooers, Christine S.; Janghorbani, Morteza

CS Clin. Nutr. Res. Cent., Univ. Chicago, Chicago, IL, 60637, USA

SO Analyst (London) (1989), 114(6), 667-74 CODEN: ANALAO; ISSN: 0003-2654

DT Journal

LA English

AΒ

A method for the isotopic detn. of Se in biol. matrixes is described. method is based on hydride generation inductively coupled plasma mass spectrometry (ICP-MS). The development is specifically related to the requirements of stable isotope tracer studies in human subjects. method is based on isotope diln. using 82Se as the in vitro spike and can quantify the 74Se and 77Se contents of samples. It involves wet oxidn. (HNO3-H202 or HNO32-HCIO4) of the 82Se-spiked matrix, redn. to selenite by boiling with HCl followed by measurement of the isotope ratios (82Se/77Se and 74Se/77Se) in the gas stream (H2Se) generated from online redn. of the sample selenite with NaBH4. Compared with the isotopic signal resulting from a selenite soln. contg. 5 ng/mL of Se, the total sample blank isotopic signal resulting from a selenite soln. contg. 5 ng/mL of Se, the total sample blank contributions at m/z = 74, 77 and 82 were <5% of the resp. isotope signal. Worst-case abs. detection limits were 0.2-0.9 ng of Se, depending on the isotope used. Ion beam intensity ratios were measured with an over-all precision [relative std. deviation (RSD)] of 1% for both isotope pairs. Measured ratios ((MRa/b) were stable during a given day's operation within the expected precision of the measurements but varied for different days. The magnitude of MRa/b was generally independent of the nature of the matrix. Highly linear relationships were found between ion beam intensity ratios (MRa/b) and the corresponding true isotope ratios for calibration solns. whose isotope ratios had been altered by as much as 1 order of magnitude. The precision/accuracy of the isotopic anal. was established by replicate measurements of the Se content of severe biol. matrixes [National Bureau of Stds. Std. Ref. Material (NBS SRM) 1577a Bovine Liver, human plasma, red blood cells and human urine], and comparison of the results with independent measurements obtained using hydride generation at. absorption spectrometry (AAS). The following data were obtained (mean  $\pm$ SD, n = 3-5; 1st result, hydride generation ICP-MS; 2nd result, hydride generation AAS): NBS SRM 1577a Bovine Liver, 0.697 ± 0.002, 0.69  $\pm u$  0.01  $\mu g/g$ ; plasma, 0.098  $\pm$  0.001, 0.135  $\pm$  0.008  $\mu g/g$ ; red blood cells, 0.211  $\pm$  0.002, 0.216  $\pm$  0.012  $\mu g/g$ ; and urine, 0.0473  $\pm$  0.0003,  $0.0489 \pm 0.0003$  tmg/mL. It was concluded that the proposed method could be used as the measurement method for studies of Se metab. in human subjects using the concept of stable isotope tracers. Compared with other available methods of isotopic anal., this method possesses the added advantage of requiring no chem, sepn, steps as the hydride generation is sufficient for removal of any potential matrix-related interferences.

ANSWER 90 OF 153 CA COPYRIGHT 2000 ACS

109:226131 CA

AN

TI Calculation of substrate flux using stable isotopes

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Am. J. Physiol. (1988), 254 (4, Pt. 1), E526-E531 CODEN: AJPHAP; ISSN:

0002-9513

DTJournal

LA English

AΒ

The use of stable isotope tracers to calc. substrate kinetics in humans is favored over the use of radioactive isotopes because of their greater safety and versatility. However, potential complications not met when dealing with radioactive tracers are caused by (1) the natural occurrence of the stable isotope used as a tracer and (2) the necessity to administer the tracer in an amt. that cannot be treated as massless. It was desirable to derive a theor. valid equation for calcq. the rate of appearance, Ra, of a substrate under steady-state conditions using a stable isotope tracer. This theor. valid equation yields results that differ from those of the equations conventionally used to calc. (endogeneous) Ra in steady state. Quant. detn. of the error in one of these equations revealed that for tracers commonly used in metabolic studies the error is negligible, whereas the error made in the other equation is likely to be quite high in commonly encountered situations. Finally, to allow for proper use of different definitions of isotopic enrichment that have arisen from practical considerations, the results derived above were used to det. valid equations for Ra appropriate to the two prevalent definitions.

ANSWER 94 OF 153 CA COPYRIGHT 2000 ACS

108:146523

Measurement of stable isotopes of bromine in biological fluids with inductively coupled plasma mass spectrometry

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CS Dep. Med., Univ. Chicago, Chicago, IL, 60637, USA

SO Analyst (London) (1988), 113(3), 405-11 CODEN: ANALAO; ISSN: 0003-2654

DT Journal LA

ΑU

AB

English A method is reported for the accurate measurement of the two stable isotopes of bromine in biol. fluids of interest in human metabolic studies. The method is based on inductively coupled plasma mass spectrometry It is shown that the background ion beam intensities at m/z = 79and 81 are typically in the range 70-335 and 600-7200 ions/s, resp., when de-ionized water is aspirated into the plasma. The corresponding range for 1.0  $\mu$ g/mL of natural Br is 9700-18,500 ions/s at m/z = 79. The detection limit  $(3\sqrt{B})$  for Br is in the range 2-5 ng/mL. A method is given for automatic correction of the argon contribution at m/z = 81. Data are presented which show that the isotope ratio 81Br/79Br can be measured routinely with a precision (relative std. derivation) of 1% or better. The measured ratio is independent of the Br concn. in the range 3-20  $\mu g/mL$ . Linear regression equations are obtained for stable isotope calibration graphs over the range 0.997-5.322 (MIR81/79). However, the slopes of these plots deviate considerably from the expected value of one. Two chem. sepn. schemes are described, Scheme I, based on cation exchange and Scheme II, based on distn. from acidified solns. The former is applicable to plasma (and possible saliva) samples whereas the latter is successful for urine. The presence of large amts. of sulfate produces significant enhancement of the ion intensity at m/z = 81 (due to 32S16O31H+). Distn. permits the required sepn. of Br from sulfate, whereas pptn. with Ba(NO3)2 does not appear to be satisfactory. Application of the method of std. addns. and stable isotope diln. anal. to samples of urine from several subjects indicates that this method permits quant. anal. of bromine to be carried out with a precision (and accuracy) of about 2%.

LAY ANSWER 98 OF 153 CA COPYRIGHT 2000 ACS

AN 105:126166 CA

Inductively coupled plasma mass spectrometric detection for multielement flow injection analysis and elemental speciation by reversed-phase liquid chromatography

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CS Dep. Chem., Iowa State Univ., Ames, IA, 50011, USA

SO Anal. Chem. (1986), 58(12), 2541-8 CODEN: ANCHAM; ISSN: 0003-2700

DT Journal

LA English

The feasibility of using an inductively coupled plasma mass spectrometer as AΒ a multielement detector for flow-injection anal. (FIA) and ion-pair reversed-phase liq. chromatog. was investigated. Sample introduction was by ultrasonic nebulization with aerosol desolvation. Abs. detection limits for FIA ranged from 0.01 to 0.1 ng for most elements using  $10-\mu L$ injections. Over 30 elements were surveyed for their response to both anionic and cationic ion pairing reagents. The sepn. and selective detection of various As and Se species were demonstrated, yielding detection limits near 0.1 ng (as element) for all 6 species present. Detn. of 15 elements in a single injection with multiple ion monitoring produced similar detection limits. Isotope ratios were measured with sufficient precision (better than 2%) and accuracy (~1%) on eluting peaks of Cd and Pb to demonstrate that liq. chromatog./inductively coupled plasma mass spectrometry should make speciation studies with stable tracer isotopes feasible.

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